

Vacuum energy and θ -vacuum

M. Asorey ^a

^aDepartamento de Física Teórica, Facultad de Ciencias
Universidad de Zaragoza, 50009 Zaragoza, Spain

The highly non-trivial structure of the θ -vacuum encodes many of the fundamental properties of gauge theories. In particular, the response of the vacuum to the θ -term perturbation is sensitive to the existence of confinement, chiral symmetry breaking, etc. We analyze the dependence of the vacuum energy density on θ around two special values, $\theta = 0$ and $\theta = \pi$. The existence or not of singular behaviors associated to spontaneous breaking of CP symmetry in these vacua has been a controversial matter for years. We clarify this important problem by means of continuum non-perturbative techniques. The results show the absence of first order cusp singularities on the vacuum energy density at $\theta = 0$ and $\theta = \pi$ for some gauge theories. This smooth dependence of the energy on θ might have implications for long standing cosmological problems like the baryonic asymmetry and the cosmological constant problem.

1. Introduction

In four-dimensional space-times non-abelian gauge theories exhibit a highly non-trivial vacuum structure. A non-perturbative condensation of classical configurations carrying special topological properties (monopoles, vortices, instantons) provides a adequate medium for the confinement of fundamental fermions. The special topological properties of non-abelian groups and the dimensionality of space time make also possible the appearance of a twist in the tunneling properties of the vacuum. This twist of the vacuum can be explicitly induced by the introduction in the action of a term proportional to the topological charge of the classical gauge fields. However, since this term breaks CP invariance there are severe constraints in the value of its θ -coefficient. In particular, the absence of a significant electric dipolar momentum of the neutron requires that $\theta < 10^{-9}$ [1].

There are two cosmological parameters with similar extremely small values: the baryon asymmetry ($\eta = N_B/N_\gamma \leq 10^{-10}$) which measures the ration of the number of baryons to the number of photons of the Universe, and the cosmological constant Λ which although very small ($\Lambda/(M_P^2) \leq 10^{-122}$) plays a fundamental role in

the acceleration of the expansion of the Universe [2]. The unnatural smallness of these parameters has puzzled cosmologists and particle physicists for a long time [3].

In the last few years there has been an increasing interest on the solution of these longstanding cosmological problems. Some proposals based on the structure of the θ vacuum have been recently formulated [4]. In these scenarios the cosmological constant value and the baryonic asymmetry are associated to the tunneling between different classical vacua of a Yang-Mills like theory. The vacuum energy is assumed to vanish for some value of θ but the crucial assumption is that the initial state of the Universe is instead of this θ -vacua a state localized around a classical vacua. The tunneling from this initial state to θ -vacuum is exponentially suppressed and might account for the tiny value of the present cosmological constant [4] and the observed baryonic asymmetry [5]. According to this picture the value of the cosmological constant will decrease with the time evolution of the Universe. Although the approach is very appealing it suffers from inconsistency. Gauge invariance implies that all classical vacua are equivalent, thus, localization around one specific vacua requires the breaking of gauge invariance. On the other the existence of a finite

mass gap requires that any physical state with very small energy must involve a fine-tuning of the coefficients of the series expansion of the state in stationary states.

From a different perspective a more conservative approach simply remarks the common smallness of the three parameters (QCD θ parameter, the cosmological constant and the baryonic asymmetry) and suggests that there might exist a relation between them. One appealing feature of this scenario is that three fundamental fine tuning problems are reduced to only one. Although one has still to explain the reason for the existence of the common fine tuning.

There are extra reasons to suspect that θ is connected with the other two cosmological parameters. In fact, the mere existence of a non-trivial value of $\theta \neq 0$ has dramatic consequences for both cosmological problems. In all approaches to the solution of the baryonic asymmetry problem the requirement of violation of CP symmetry appears as a fundamental prerequisite. Although there are other leading sources of CP violation the possibility of having a non-trivial θ -vacuum is a complementary signal of the existence of the asymmetry.

The variation of the vacuum energy with θ also opens the possibility of a connection with the cosmological constant problem. If the cosmological constant vanishes for some value of θ (e.g. $\theta=0$) by some fundamental reason or theory (strings, supersymmetry, quantum gravity, etc), an infinitesimal deviation of value of θ might induce a very tiny vacuum energy density enough to explain the small observed value of Λ . However, the constraint imposed on θ by the current bounds on the electric dipolar momentum of the neutron are not enough to accommodate the smallness of the cosmological constant. Indeed if we assume that the dependence of the vacuum energy on θ is analytic around $\theta=0$ the vacuum energy density \mathcal{E}_θ of θ -vacuum is given by $\mathcal{E}_\theta = \mathcal{E}_0 + c \theta^2 + \mathcal{O}(\theta^4)$, where the coefficient c is proportional to the inverse of the mass of the lightest quark Λ^6/m_u^2 . For $\theta < 10^{-9}$ we obtain a bound $\mathcal{E} = \mathcal{E}_\theta - \mathcal{E}_0 < 10^{-22} \text{ GeV}^4$ which is much higher than the cosmological bound $\mathcal{E} < 10^{-47} \text{ GeV}^4$. Although the estimate is very rough the θ -vacuum scenario re-

quires to the bound on the value of θ to be more stringent $\theta < 10^{-21}$ than that provided by the current measures of the electric dipolar structure of the neutron. The estimate is based on the assumption that the vacuum energy density \mathcal{E}_θ has a smooth dependence on θ which generically implies a lower variation of the vacuum energy density.

The smoothness of \mathcal{E}_θ is claimed to hold at first order around $\theta=0$ by the Vafa-Witten theorem [6] on the absence of spontaneous symmetry breaking of CP symmetry in QCD. However, some doubts have been recently raised about the validity of the Vafa-Witten proof of the theorem [7–10]. In fact, \mathcal{E}_θ is not always smooth at $\theta=\pi$: there are cases where CP is spontaneously broken at that point. In principle, the same pathology could appear also at $\theta=0$.

If we assume that \mathcal{E}_θ has a smooth behavior at $\theta=0$ and $\theta=\pi$ a very simple argument shows that the expectation value of the topological density

$$\mathcal{E}'_\theta = -\frac{i}{16\pi^2} \langle F_{\mu\nu} \tilde{F}^{\mu\nu} \rangle_\theta$$

vanishes at $\theta=0$ and $\theta=\pi$, i.e. $\mathcal{E}'_{\theta=0} = \mathcal{E}'_{\theta=\pi} = 0$. The argument is based on the fact that the two classically CP symmetric vacua $\theta=0$ and $\theta=\pi$ are extremal points of the vacuum energy density. In the case $\theta=0$ this property follows from reflection CP symmetry $\mathcal{E}_\theta = \mathcal{E}_{-\theta}$ which implies that \mathcal{E}_θ has a local extrema (maximum or minimum) at $\theta=0$. In the case $\theta=\pi$ the same property follows from Bragg symmetry $\mathcal{E}_{\pi+\theta} = \mathcal{E}_{\pi-\theta}$, which is a consequence of CP symmetry and θ -periodicity $\mathcal{E}_\theta = \mathcal{E}_{\theta+2\pi}$. Thus, if \mathcal{E}_θ is smooth its first derivative and the vacuum expectation value of the topological density vanish at $\theta=0$ and $\theta=\pi$. The vanishing of this order parameter of CP symmetry is natural because the smoothness \mathcal{E}_θ is equivalent to the absence of first order phase transition and therefore compatible with the absence of spontaneous breaking.

Thus, the search for the smoothness of \mathcal{E}_θ around the points $\theta=0$ and $\theta=\pi$ becomes in fact a search of spontaneous breaking of CP symmetry. In this paper we further clarify the presence or not of cusp singularities in \mathcal{E}_θ around the 0-vacuum and π -vacuum. Among the four

possible scenarios with possible cusps in any of the CP symmetric vacua (Fig. 1) we will find that QCD realizes the maximally smooth behavior without cusps (Fig. 1(d)).

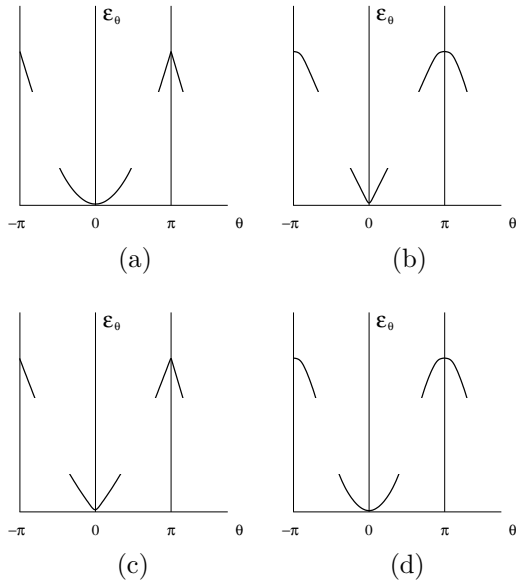


Figure 1. Four different scenarios for possible behaviors of the vacuum energy density \mathcal{E}_θ . In the first case (a) the cusp at $\theta = \pi$ signals the spontaneous breaking of CP symmetry in π -vacuum. In case (b) CP symmetry is broken at $\theta = 0$ but the π -vacuum is CP invariant. In the third case (c) there are two cusps at $\theta = \pi$ and $\theta = 0$ meaning that none of those vacua is CP invariant. Finally, in case (d) \mathcal{E}_θ is smooth and CP symmetry is preserved for both values of θ .

2. Vafa-Witten theorem

The Vafa-Witten theorem is one of the very few non-perturbative analytic results of QCD. It provides a strong constraint on the behavior of the vacuum energy density \mathcal{E}_θ for small values of θ -parameter. A very simple and elegant argument pointed by Vafa and Witten [6] shows why spontaneous violation of parity symmetry is not present in QCD and in any gauge theory with Dirac fermions in 3+1 space-time dimensions. This result implies, in particular, that the expectation value of the topological density vanishes in the $\theta = 0$ vacuum. The argument exploits the positivity of the Yang-Mills Euclidean measure [11,12] and fermionic determinants [6] which

implies the existence of a real effective action

$$S_{\text{eff}}(g) = \frac{1}{2g^2} \int F_{\mu\nu} F^{\mu\nu} - \log \det(\not{D} + m)$$

and an upper bound for partition function of the θ -vacuum

$$\mathcal{Z}_\theta = \int \delta A e^{-S_{\text{eff}}(g) + \frac{i\theta}{16\pi^2} \int F_{\mu\nu} \tilde{F}^{\mu\nu}} < \mathcal{Z}_0 \quad (1)$$

in terms of the 0-vacuum partition function. Notice that the partition function \mathcal{Z}_θ is always real because CP symmetry transforms $F\tilde{F}$ into $-F\tilde{F}$ and preserves the effective gauge action $S_{\text{eff}}(g)$. The inequality (1) implies that the free energy density $\mathcal{E}_\theta = E_\theta/V$ of the θ -vacuum is bounded below by that of the 0-vacuum, i.e. $\mathcal{E}_0 \leq \mathcal{E}_\theta$; from this property Vafa-Witten argued implicitly assuming that \mathcal{E}_θ is smooth at $\theta = 0$ that $\mathcal{E}'_0 = \langle F\tilde{F} \rangle_0 = 0$. A criticism recently raised to the Vafa-Witten proof objects that the very existence of a first order phase transition might imply that the vacuum energy density or the free energy is not well defined [7] and, thus, the Vafa-Witten argument will be invalid. However, in this case there is no doubt about the existence of a well defined free energy for any real value of the θ parameter. This is guaranteed by unitarity of the theory, which is translated into Osterwalder-Schrader (OS) positivity of the Euclidean functional measure of the theory with real θ -terms [13,14]. This special property of Yang-Mills theory excludes the possibility that pathological scenarios where the free energy is ill-defined [7] might occur in the theory. However, this fact does not mean that the theorem is already proven. One needs to exclude the existence of a cusp in the energy density at $\theta = 0$. The appearance of the cusp would signal the existence of a first order phase transition and spontaneous breaking of parity at $\theta = 0$ without violation of the Vafa-Witten inequality for free energies. The only extra property one needs to prove is smoothness of \mathcal{E}_θ at $\theta = 0$, which would make the existence of such a cusp not possible. In other terms, $\theta = 0$ is always an absolute minimum of the free energy density but only if \mathcal{E}_θ is smooth we will have $\mathcal{E}'_0 = 0$. Only in that case one can make sure that the vacuum

expectation value of the topological density vanishes and the Vafa-Witten theorem holds for this particular order parameter. The smoothness of \mathcal{E}_θ at $\theta = 0$ has been first proved in Ref.[15]. Let us summarize the essential arguments of the proof.

3. Analytic Continuation and Lee-Yang's zeros

The proof is based on the analysis of possible existence of Lee-Yang singularities. Non-analyticities in the θ dependence can be easily traced from the lack of an analytic continuation into the complex θ plane. Indeed, for complex values of θ OS positivity (i.e. unitarity) is not preserved and there is no guarantee that the free energy is well defined, in which case it does not make sense to speak about smoothness. Essentially, there are two possible ways in which the θ theory might give rise to pathological non-analyticities in the complex sector. One possibility is that the analytic continuation of the partition function for complex values of θ is not defined at all, i.e. the partition function itself becomes divergent. The other possibility is that the partition function exhibits a sequence of zeros converging to $\theta = 0$ in the infinite volume limit. This is the scenario advocated by Lee and Yang [16] which signals in many cases the existence of a phase transition.

For complex values of θ the partition function can be split into a sum of functional integrals over the different topological sectors

$$\mathcal{Z}_\theta(g) = \sum_{q=-\infty}^{\infty} e^{-q \text{Im } \theta + i q \text{Re } \theta} \int_{c_2(A)=q} \delta A e^{-S_{\text{eff}}(g,q)}$$

In a strict sense, the functional integral is UV divergent but it can be regularized in such a way that its positivity properties are preserved [12]. We can consider such a geometrical regularization whenever it is required. On the other hand, in the infinite volume limit $\mathcal{Z}_\theta(g)$ vanishes unless the vacuum energy is renormalized to 0. But it is just the dependence on θ of the vacuum energy what we want to analyze. Therefore, we will consider throughout this note a compact space-time with large but finite volume $VT < \infty$.

On the other hand the θ -term of the action is

bounded above by the Yang-Mills action $S_{\text{YM}}(q)$ in every q -topological sector by the BPS bound $S_{\text{YM}}(g,q) \geq 4\pi^2|q|/g^2$. In the regularized theory, the coefficient of this linear bound increases with the UV regulating scale. In general, from positivity of fermionic determinants, Yang-Mills measure and the BPS bounds we have the inequality

$$\begin{aligned} |\mathcal{Z}_\theta(g)| &\leq \sum_{q=-\infty}^{\infty} e^{q \text{Im } \theta} \int_{c_2(A)=q} \delta A e^{-S_{\text{eff}}(g,q)} \\ &\leq \sum_{q=-\infty}^{\infty} \int_{c_2(A)=q} \delta A e^{-S_{\text{eff}}(\tilde{g},q)} = \mathcal{Z}_0(\tilde{g}) \end{aligned}$$

where $1/\tilde{g}^2 = 1/g^2 - |\text{Im } \theta|/4\pi^2$. This shift of the gauge coupling constant can be considered as a change of the renormalization point. This shows that the partition function of the original theory with a complex θ -term is bounded by the partition function of a similar theory with $\theta = 0$ but with a different coupling constant. Since the theory at $\theta = 0$ is unitary and renormalizable, its partition function \mathcal{Z}_0 is finite and from the above inequality it follows that $|\mathcal{Z}_\theta| < \infty$ is also finite for small values of $\text{Im } \theta$. If in addition the theory is asymptotically free, then the renormalization of g^2 in the UV fixed point can absorb any value of $\text{Im } \theta$, which implies an infinite radius of convergence of the sum over topological sectors in the complex θ plane. To make the argument more precise one should consider the regularized theory. The bare coupling constant g has to be fine tuned according to the renormalization group to yield the appropriate continuum limit. But because of asymptotic freedom this coupling goes to zero as the UV regulator is removed and the shift from g to \tilde{g} induced by $\text{Im } \theta$ simply implies a change in the effective scale of the continuum theory.

The only remaining possible source of non-analyticity is the presence of Lee-Yang singularities, i.e. zeros in the partition function \mathcal{Z}_θ which could prevent the existence of a unique limit of the free energy $\log \mathcal{Z}_\theta$ or its derivatives at $\theta = 0$. Uniform convergence of the sum over topological sectors implies continuity of \mathcal{Z}_θ on the complex. Now, since $\mathcal{Z}_\theta > 0$ for finite space-time volumes and real values of θ , from 2π -periodicity of \mathcal{Z}_θ and

compactness of $[0, 2\pi]$ follows the existence of an open strip covering the real θ -axis where $\mathcal{Z}_\theta \neq 0$. This implies that for finite volumes there is no phase transition for any real value of θ . However, in the infinite volume limit $\mathcal{Z} \searrow 0$ as $V \nearrow \infty$ and the argument does not provide information about the critical behavior of the theory.

Now, the positivity argument of Vafa and Witten can be used to show the absence of Lee-Yang zeros for pure imaginary values of θ in vector-like gauge theories. Indeed, if θ is purely imaginary $\theta = i\vartheta$, the contribution of every topological sector is positive ($\text{Re } \theta = 0$) and the full partition function is real and strictly positive ($\mathcal{Z}_{i\vartheta} > 0$), i.e. $\mathcal{Z}_{i\vartheta}$ has no Lee-Yang zeros for any value of ϑ . This property is essential for the proof parity symmetry cannot be spontaneously broken.

The partition function \mathcal{Z}_θ can be split into two terms $\mathcal{Z}_\theta = \mathcal{Z}_\theta^+ + \mathcal{Z}_\theta^-$, encoding the contributions of parity even (\mathcal{Z}_θ^+) and parity odd (\mathcal{Z}_θ^-) states. In the physical θ -sector ($\text{Im } \theta = 0$), \mathcal{Z}_θ^\pm are defined by $\mathcal{Z}_\theta^\pm = \frac{1}{2}\mathcal{Z}_\theta \pm \frac{1}{2}\mathcal{Z}_\theta^P$, where \mathcal{Z}_θ^P is given by $\text{Tr } P e^{-TH_{\theta+2\pi}}$ in terms of the Hamiltonian $H_{\theta+2\pi}$ and parity operator P . For general values of θ , \mathcal{Z}_θ^P is given by the standard functional integral \mathcal{Z}_θ but with the θ parameter shifted to $\theta + 2\pi$ and parity odd boundary conditions $A(-T/2) = [A^P(T/2)]^\phi$, where ϕ is any gauge transformation and $A^P(T/2)$ is the parity transform of $A(T/2)$, i.e. $A^P(T/2) = (A_0^P(T/2), A_i^P(T/2))$ with $A_0^P(\vec{x}, T/2) = A_0(-\vec{x}, T/2)$, $A_i^P(\vec{x}, T/2) = -A_i(-\vec{x}, T/2)$ [6]. The functional integral approach provides an explicit analytic continuation of \mathcal{Z}_θ^P , \mathcal{Z}_θ^+ and \mathcal{Z}_θ^- to the complex domain $|\text{Im } \theta| < \theta_c$. Since $\mathcal{Z}_\theta > 0$ for any real or imaginary value of θ in finite volumes, by continuity there exists an open domain in the θ -plane covering the real and imaginary axis which is free of Lee-Yang zeros for \mathcal{Z}_θ and \mathcal{Z}_θ^\pm . In that domain \mathcal{Z}_θ^\pm can be rewritten as $\mathcal{Z}_\theta^\pm = e^{-\xi_\pm(\theta)}$ in terms of two analytic functions $\xi_+(\theta)$ and $\xi_-(\theta)$.

If there were a first order phase transition at $\theta = 0$ with spontaneous parity symmetry breaking the expectation value of the CP breaking order parameter

$$-\frac{i}{16\pi^2} \left\langle F_{\mu\nu} \tilde{F}^{\mu\nu} \right\rangle_{\theta=0}^- = \lim_{VT \rightarrow \infty} \frac{\xi'_-(\theta)}{VT} \Big|_{\theta=0}$$

$$= \frac{i}{16\pi^2} \left\langle F_{\mu\nu} \tilde{F}^{\mu\nu} \right\rangle_{\theta=0}^+ = - \lim_{VT \rightarrow \infty} \frac{\xi'_+(\theta)}{VT} \Big|_{\theta=0} \neq 0$$

would not vanish. Since $\mathcal{Z}_\theta(g)$ is real for imaginary values of $\theta = i\vartheta$ the existence of a cusp associated to level crossing would imply that, $\xi_-(i\vartheta)^* = \xi_+(i\vartheta)$ and

$$\mathcal{Z}_{i\vartheta} = 2e^{-\text{Re } \xi_+(i\vartheta)} \cos \text{Im } \xi_+(i\vartheta).$$

Now, the CP symmetry breaking condition requires that $\text{Im } \xi_+(i\vartheta)$ be unbounded for imaginary values of $\theta = i\vartheta$ close to $\vartheta = 0$ in the infinite volume limit. This fact implies that if the system undergoes a first order phase transition with parity symmetry breaking an increasing number of Lee-Yang zeros must arise in the partition function \mathcal{Z}_θ for imaginary values of θ and large enough volumes. The localization of zeros in the unit circle $|w| = 1$ of the complex plane $w = e^{i\theta}$ is reminiscent of the Lee-Yang theorem for spin systems [16]. However this cannot occur in vector-like gauge theories where we have shown that for any finite volume the partition function \mathcal{Z}_θ has no zeros on the imaginary line $\text{Re } \theta = 0$. Therefore, the system cannot undergo a first order phase transition at $\theta = 0$ with parity symmetry breaking. In other terms, there is not a first order cusp in the vacuum energy density \mathcal{E}_θ at $\theta = 0$, i.e. $\mathcal{E}'_0 = 0$ and the Vafa-Witten theorem holds.

The existence of any odd-order phase transition can be discarded for the same reason because the function $\text{Im } \xi_+(i\vartheta)$, which is odd in ϑ , would be unbounded and \mathcal{Z}_θ would have Lee-Yang zeros for some values of $\theta = i\vartheta$. However, even-order phase transitions cannot be excluded by these arguments because such transitions will not require spontaneous parity symmetry breaking. Recent numerical estimates provide some evidence on the absence of second order transitions for a large family of gauge groups [17].

In summary, there is now a complete proof of the first order smoothness of the vacuum energy density at $\theta = 0$: the missing link in the Vafa-Witten argument about the vanishing of the topological charge order parameter.

4. π -vacuum

From the above arguments we cannot, however, exclude the existence of first order phase transitions for other values of $\theta \neq 0$. In particular, we cannot discard the existence of CP symmetry breaking for $\theta = \pi$. Some authors claim the existence of a sharp first order transition at $\theta = \pi$ associated to spontaneous symmetry breaking of CP [18–21] induced by massive quarks. In that case, the analytic continuation of the partition function \mathcal{Z}_θ to complex values of θ becomes an oscillating series and there might exist values of ϑ as close as possible to $\vartheta = 0$ where the partition function $\mathcal{Z}_\theta = 0$ vanishes. However, in pure Yang-Mills theory or theories with different quark masses some arguments support a CP symmetry preserving scenario for the $\theta = \pi$ vacuum. They are based on the existence of a strong level repulsion between parity even and parity odd lowest energy states [22]. The existence of such a mechanism can be derived from the analysis of the nodal structure of the vacuum functional of $\theta = \pi$ theory. The study of nodal structure of vacuum functionals in quantum gauge theories was initiated by Feynman [23]. He argued that confinement in $2 + 1$ dimensional Yang-Mills theories is a consequence of the absence of nodes and some extra properties of the vacuum.

Standard minimum principle arguments disfavor the appearance of nodes in vacuum states of Quantum Theories [23]. However, the presence of CP violating interactions invalidates the use of such arguments and the vacuum response to this kind of interactions can involve the appearance of nodes. In some cases, the infrared behavior of the theory is so dramatically modified by the CP violating interaction that a confining vacuum state can become non-confining. The connection between the absence of confinement and the existence of nodes in the vacuum state, suggests that new classical field configurations related to the nodal structure of the quantum vacuum emerge as new candidates to play a significant role in the mechanism of confinement. This idea has been successfully exploited to show the absence of spontaneous breaking of CP symmetry at $\theta = \pi$ for various field theories [22] [24].

In the canonical formalism and Schrödinger representation the physical states of the Yang-Mills theory for any value of θ are wave functionals $\psi([A])$ defined on the gauge orbit space \mathcal{M} . This is a consequence of Gauss law. There is no topological reason to force physical states to present nodal configurations, i.e. gauge orbits where the corresponding wave functionals vanish. However, there is a very simple dynamical argument showing that for any stationary state, including the θ -vacuum, there exists a physical state with nodal configurations.

The non-trivial effect of the θ -term is due to the non-simply connected character of the orbit space $\pi_1(\mathcal{M}) = \mathbb{Z}$ or what is equivalent the non-connected character of the group of gauge transformations $\pi_0(\mathcal{G}) = \mathbb{Z}$. It is possible, however, to perform a multivalued transformation of physical states

$$\xi(A) = e^{-\frac{i\theta}{2\pi}C_s(A)}\psi_{\text{ph}}([A]) \quad (2)$$

with

$$C_s(A) = \frac{1}{4\pi} \int \text{tr} \left(A \wedge dA + \frac{2}{3} A \wedge A \wedge A \right),$$

which removes the θ dependence of the Hamiltonian

$$H_\theta = -\frac{g^2}{2} \left\| \frac{\delta}{\delta A} - \frac{i\theta}{8\pi^2} * F(A) \right\|^2 + \frac{1}{2g^2} \|F(A)\|^2$$

$$\tilde{H}_\theta = e^{-\frac{i\theta}{2\pi}C_s(A)} H_\theta e^{\frac{i\theta}{2\pi}C_s(A)} = H_0.$$

The transformation becomes single valued when restricted to the open dense subset $\mathcal{N} = \{[A] \in \mathcal{M}; C_s(A) \neq (2n+1)\pi\}$, of the orbit space \mathcal{M} . The θ dependence is encoded in the non-trivial boundary conditions that the new wave functionals ξ satisfy at the boundary of \mathcal{N} :

$$\xi(A_+) = e^{-i\nu(\phi)\theta}\xi(A_-) \quad (3)$$

for any pair of gauge fields A_- and A_+ in the same orbit of $\mathcal{M} \setminus \mathcal{N}$ which are gauge equivalent $A_+ = A_-^\phi$ by means of a gauge transformation with winding number $\nu(\phi)$. In this sense the transformation (2) is trading the θ -dependence

of the Hamiltonian by non-trivial boundary conditions on $\mathcal{M} \setminus \mathcal{N}$.

There are physically interesting configurations in this boundary domain, e.g. sphalerons. Sphalerons are static solutions of Yang-Mills equations which by Derrick theorem can only exist for finite space volumes. They are unstable and become characterized by the existence of a finite number of unstable decaying modes. The value of the Yang-Mills functional on them marks the height of the potential barrier between classical vacua and, therefore, it is related to the transition temperature necessary for the appearance of direct coalescence between those vacua. Their existence was predicted by Manton [25] by an argument based on the non-simply connected nature of the orbit space of 3-dimensional gauge fields and a generalization of the Ljusternik-Snierelman theory. An explicit expression for the sphaleron on S^3 can be obtained from the observation that the pullback of one instanton to a 3-dimensional sphere embedded on S^4 with origin on the center of the instanton and the same radius that the instanton is an unstable critical point of the 3-dimensional Yang-Mills functional. For $SU(2)$ the sphaleron in stereographic coordinates reads [26]

$$A_j = \frac{4\rho(4\rho\epsilon_{jk}^a x^k - 2x^a x_j + [x^2 - 4\rho^2]\delta_j^a)\sigma_a}{(x^2 + 4\rho^2)^2}.$$

The unstable mode can be identified with the variation of the configuration under scale transformations.

Relevant properties of sphalerons are that they give a very special value to the Chern-Simons functional $C_s(A_{\text{sph}}) = \pi$ and that they are quasi-invariant under parity transformations

$$A_{\text{sph}}^{\text{P}} = A_{\text{sph}}^{\varphi},$$

where φ denotes the gauge transformation

$$\varphi(x) = \frac{1}{x^2 + 4\rho^2} [(x^2 - 4\rho^2)I - 4i\rho x^j \sigma_j].$$

with winding number $\nu(\varphi) = 1$. In contrast, the vacuum configuration $A_{\text{vac}} = 0$ gives rise to a vanishing value for the Chern-Simons functional $C_s(A_{\text{vac}}) = 0$ and is strictly invariant under parity

$$A_{\text{vac}}^{\text{P}} = A_{\text{vac}}.$$

In the case $\theta = \pi$ the boundary condition (3) becomes an anti-periodic boundary condition $\xi(A_+) = -\xi(A_-)$ for any pair of gauge fields A_- and A_+ with $[A_-] = [A_+] \in \mathcal{M} \setminus \mathcal{N}$ which are gauge related by a gauge transformation with odd winding number. Due to the special boundary condition it is easy to see that CP parity even states must vanish on the orbits of sphaleron configurations $[A_{\text{sph}}]$ whereas that CP parity odd states vanish on the orbits of classical vacuum configurations $[A_{\text{vac}}]$. If the π -vacuum state were degenerate there will exist two different vacuum states ψ_0^+ and ψ_0^- with even and odd parities, respectively. But, since the potential term

$$V(A) = \frac{1}{2g^2} \|F(A)\|^2$$

of the Hamiltonian vanishes for the vacuum configuration whereas it gets a non-null positive value for the sphaleron gauge field, the lowest energy eigenstates ψ_0^+ and ψ_0^- cannot have the same energy. In this way the potential term induces a level repulsion which increases with space volume. The splitting of those levels means that for $\theta = \pi$ there is not spontaneous breaking of parity, the vacuum is even and vanishes for sphaleron gauge fields.

Since the theory is expected to deconfine for $\theta = \pi$, the result suggest that those nodes might be responsible for the confining properties of the vacuum in absence of θ term where the vacuum has no classical nodal configurations.

As in the case $\theta = 0$ [15] the above result shows that CP symmetry is not spontaneously broken also for $\theta = \pi$ in absence of quarks although the physical reasons are fairly different.

5. Conclusions

The above results can also be extended to other theories with similar properties. One particularly interesting case is the \mathbb{CP}^N non-linear sigma model. Indeed, from a similar analysis one can conclude that there is no spontaneous CP symmetry breaking in \mathbb{CP}^N models at $\theta = 0$ [15] and $\theta = \pi$ [24]. This result can be checked for the \mathbb{CP}^1 model where the exact solution is known for

$\theta = 0$ [27,28]. An exact solution which is parity preserving is also known for $\theta = \pi$ [29]. In both cases the exact results are in agreement with the results discussed above.

Another case where an exact solution is also known is the \mathbb{CP}^N model in the large N limit. In this case the system describes a weakly interacting and parity preserving massive scalar particle in the adjoint representation of $SU(N)$ at $\theta = 0$ and in the fundamental representation of $SU(N)$ at $\theta = \pi$. The later case has been controversial but a recent analysis [30] shows that it exhibits a behavior similar to that of Yang-Mills theory.

In conclusion, the vacuum energy density is smooth at first order for CP symmetric vacua: 0-vacuum and π -vacuum. The smooth behavior qualitatively favors cosmological applications but quantitative numerical estimates still require more stringent bounds on θ than those based on the current data of particle physics.

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